Laser Spectroscopy of Ruthenium Containing Diatomic Molecules: RuH/D and RuP

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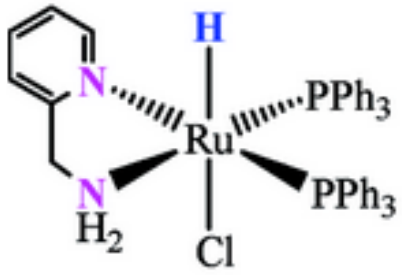
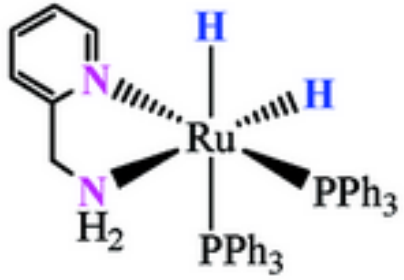
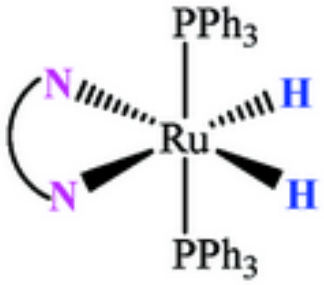
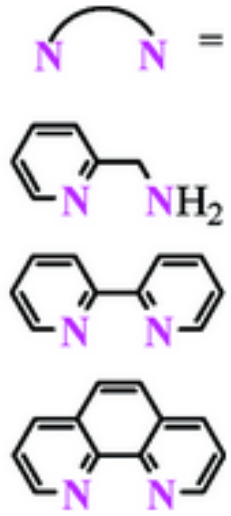
NSERC
CRSNG

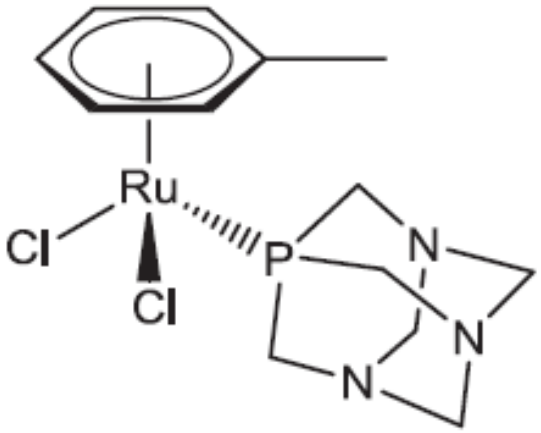
Motivation – Catalysis, Drug Design

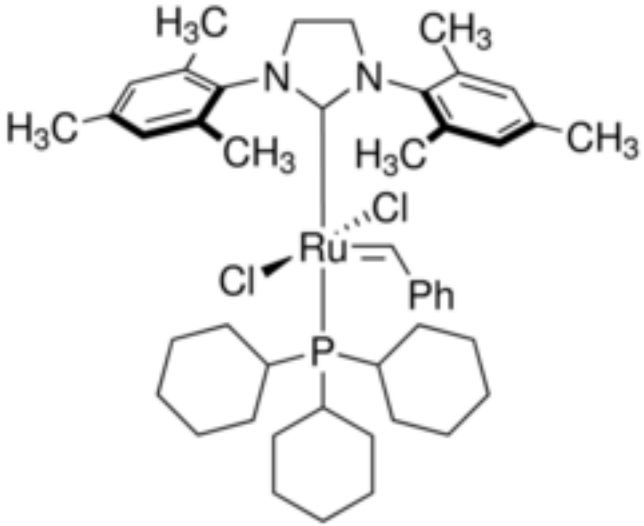








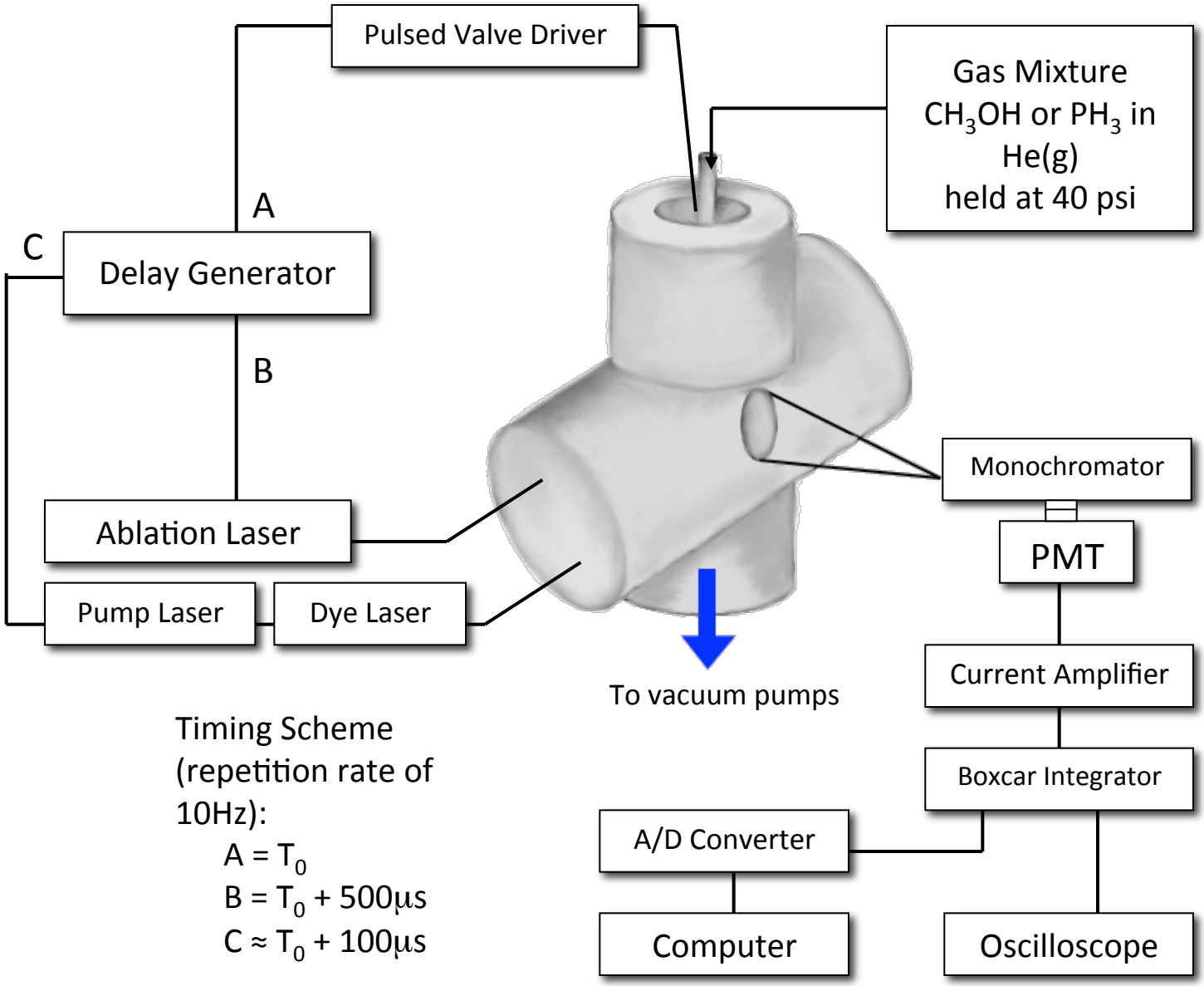




Motivation - Previous Work on Ruthenium Diatomics

- RuC: Scullman et al., Phys. Scr. 3, 19(1971), Morse et al. (1998), Steimle et al. (2003), Cheung et al. (2014).
  - $^1\Sigma^+$ from $\sigma^2\delta^4\pi^4$ configuration
- RuO: Raziunas et al., J.Chem.Phys. 43, 1010(1965), Scullman et al. (1975), Cheung et al. (2013)
  - $^5\Delta_i$ from $\delta^3\sigma^1\pi^2$ configuration
- RuN: Ram et al., J. Chem.Phys. 109, 6329(1998), Ram et al. (2002), Steimle et al. (2003)
  - $^2\Sigma^+$ from $\pi^4\delta^4\sigma^1$ configuration
- RuF: Steimle et al., J.Chem.Phys. 124, 024309(2006).
  - $^4\Phi_i$ from $\delta^3\sigma^1\pi^3$ configuration
- RuSi: Morse et al., J.Chem.Phys. 127, 084317(2007)
  - $^3\Delta_3$ from $\pi^4\delta^3\sigma^1$ configuration
- RuB: Cheung et al., Chem.Phys.Let. 547, 21(2012).
  - $^2\Delta_i$ from $\sigma^2\pi^4\delta^3$ configuration
- RuH: Balasubramanian et al., Chem. Phys.. 140, 243(1990).
  - $^4\Sigma^-$ from $\sigma^1\delta^2\pi^4$ configuration ➔ theoretical prediction
- RuP: no experiments/no theoretical predictions

Apparatus



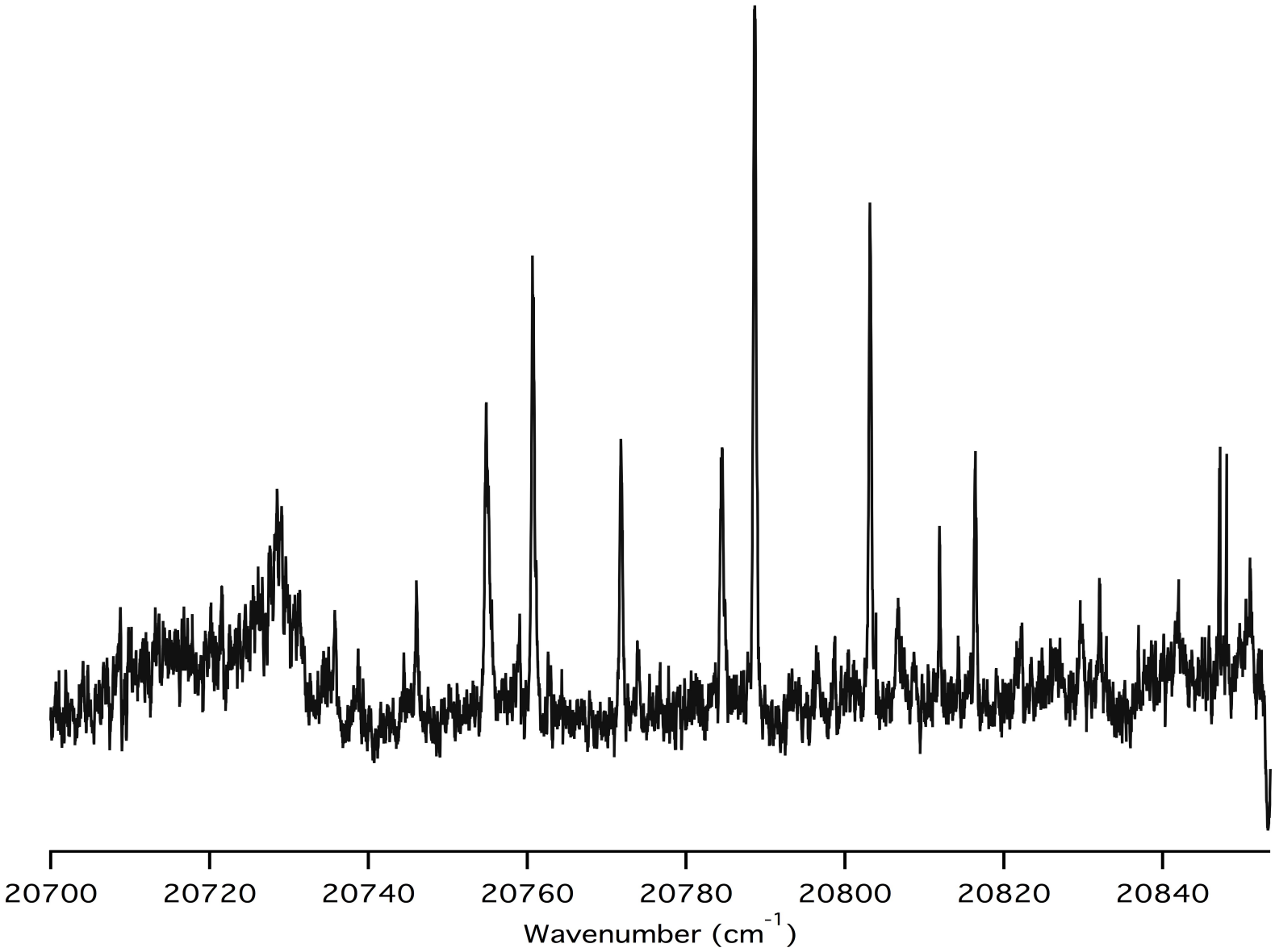
Timing Scheme (repetition rate of 10Hz):

- A = T_0
- B = T_0 + 500μs
- C ≈ T_0 + 100μs

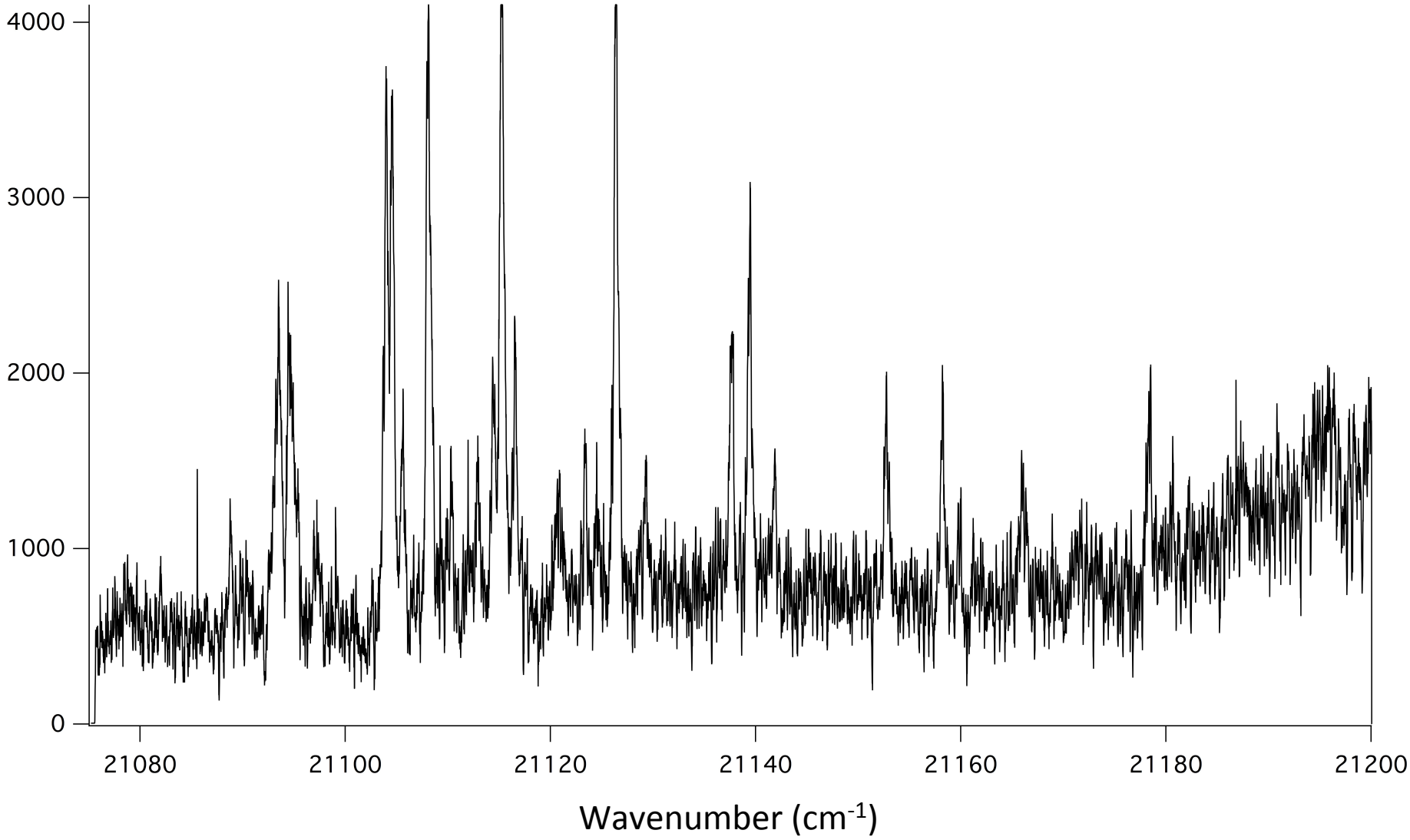
Theoretical Predictions for RuH

State	R_e (Å)	T_e (cm^{-1})	ω_e (cm^{-1})	μ_e (cm^{-1})
$^4\Sigma^-$	1.547	0	1938	2.78
$^4\Pi$	1.576	2802	1865	3.16
$^4\Phi$	1.584	2848	2075	2.76
$^4\Delta$	1.632	4748	1834	3.71
$^2\Pi$	1.550	7090	2144	2.40
$^4\Sigma^-$ (II)	1.722	11964	1441	3.63
$^4\Gamma$	1.672	18700	1827	-1.07
$^4\Pi$ (II)	1.66	18900	1791	-0.67
$^4\Delta$ (II)	1.73	22538	1658	-0.63
$^4\Sigma^+$	1.763	24000		0.36

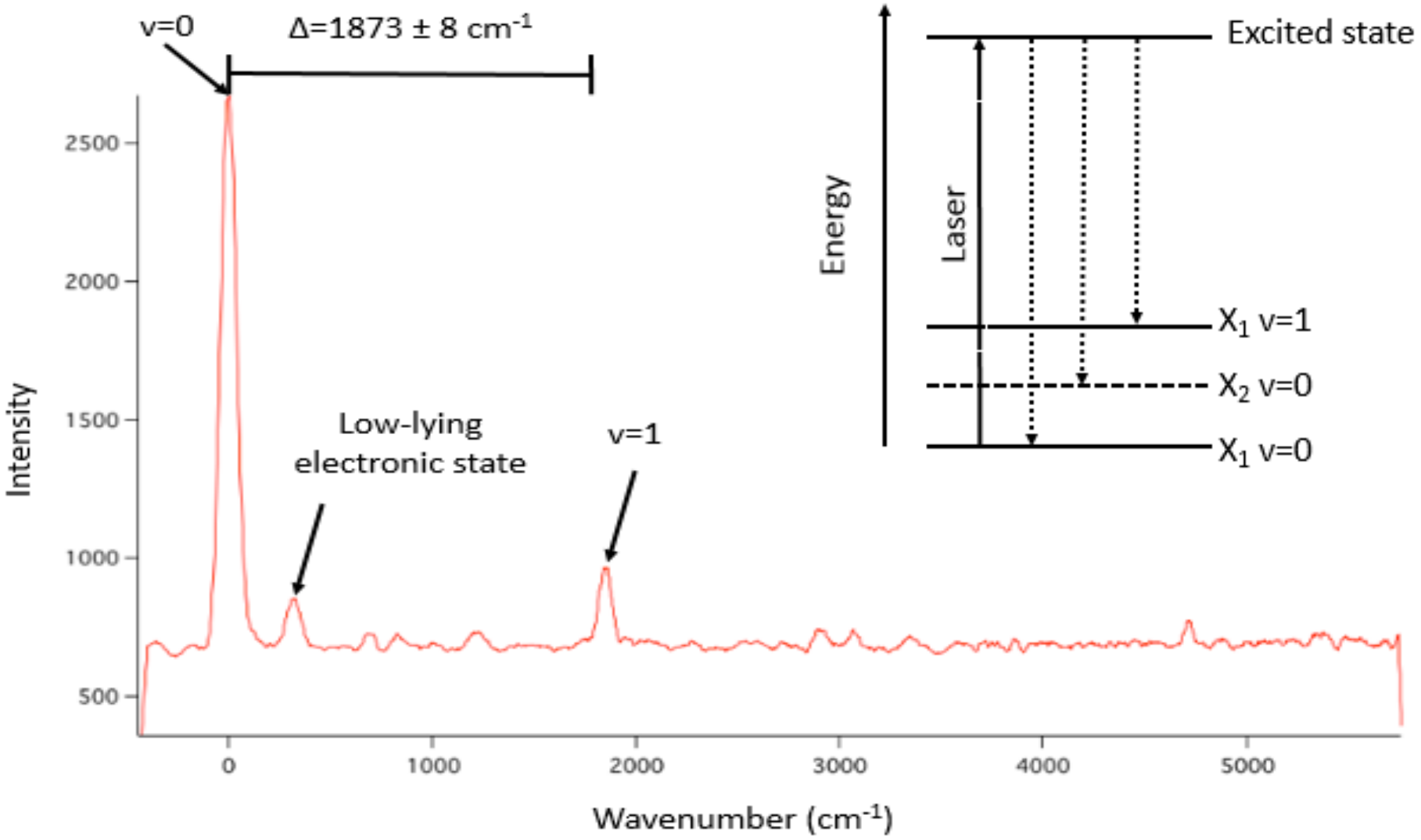
Rotationally Resolved Spectrum of RuH



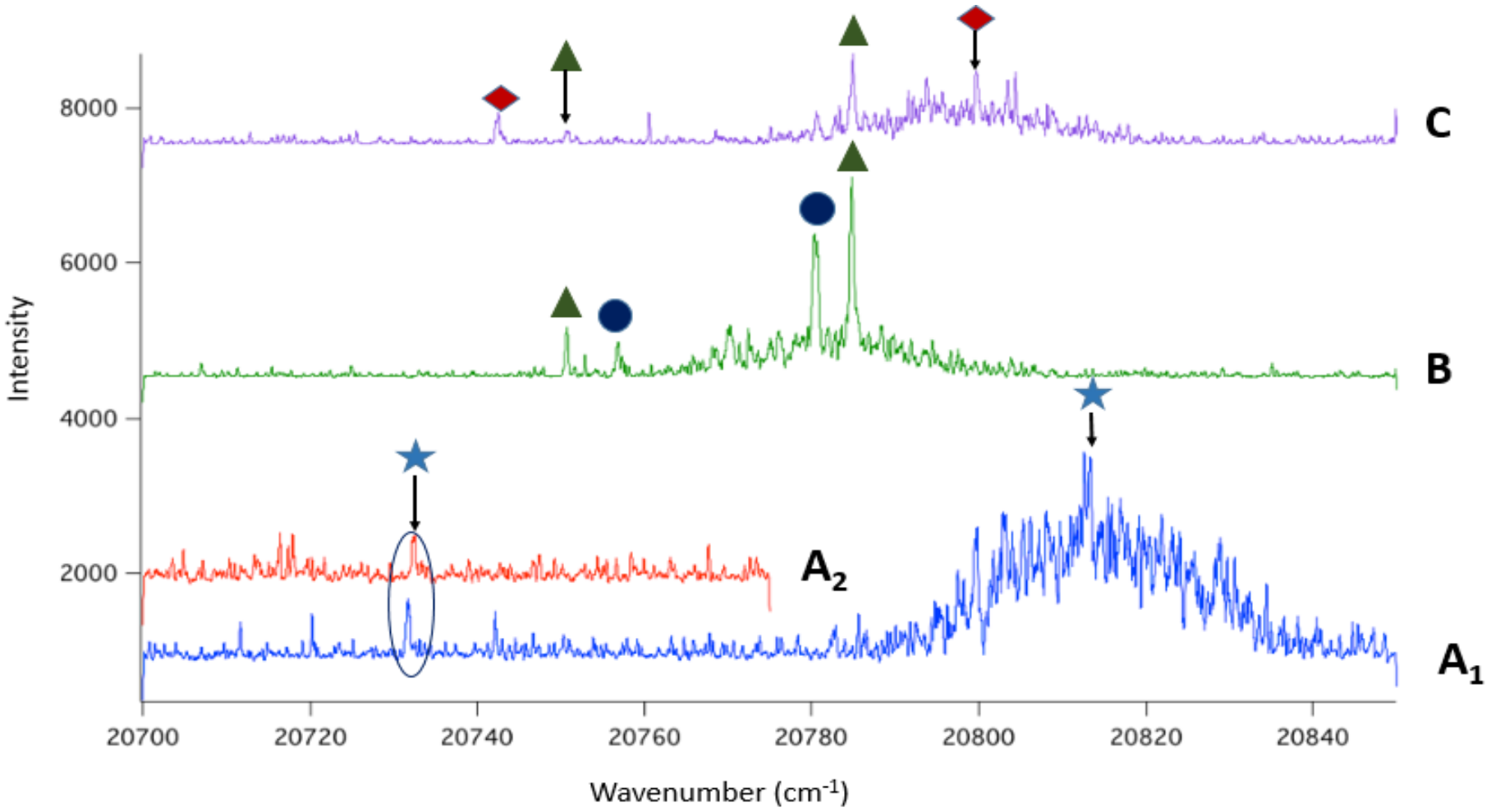
Rotationally Resolved Spectrum of RuD



Dispersed Fluorescence Spectrum of RuH

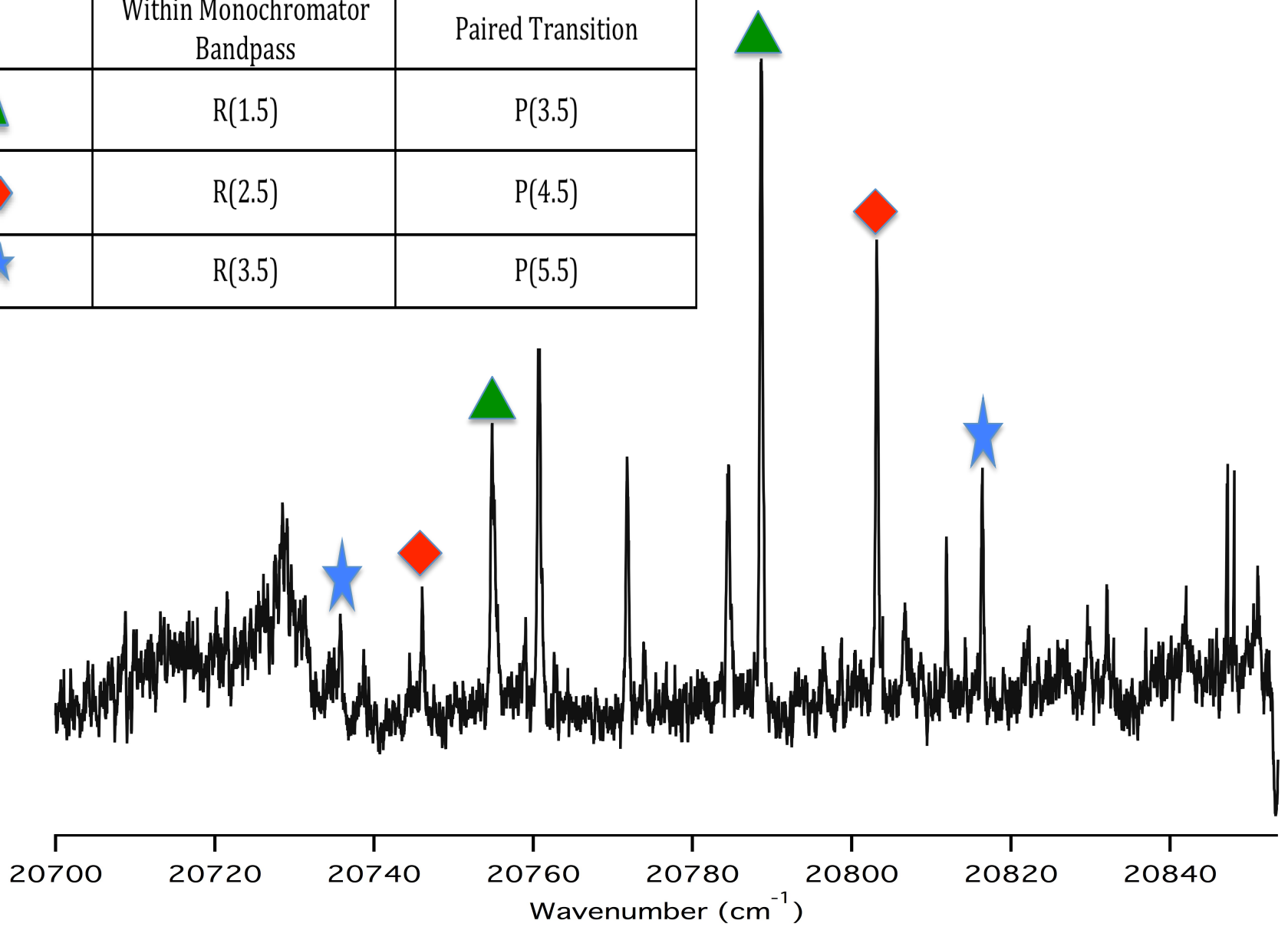


Wavelength Selective Detection

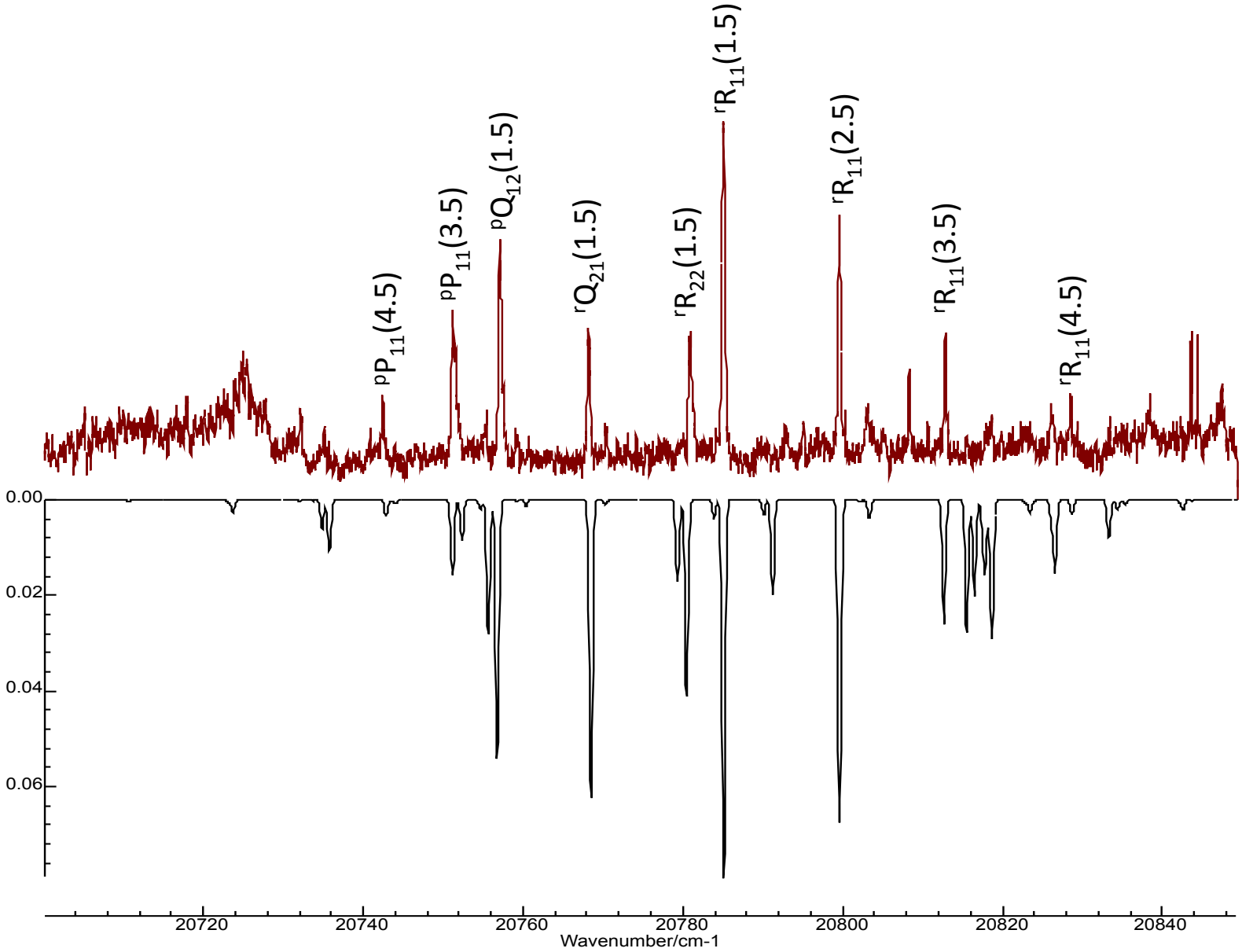


Wavelength Selective Detection

	Within Monochromator Bandpass	Paired Transition
▲	R(1.5)	P(3.5)
◆	R(2.5)	P(4.5)
★	R(3.5)	P(5.5)



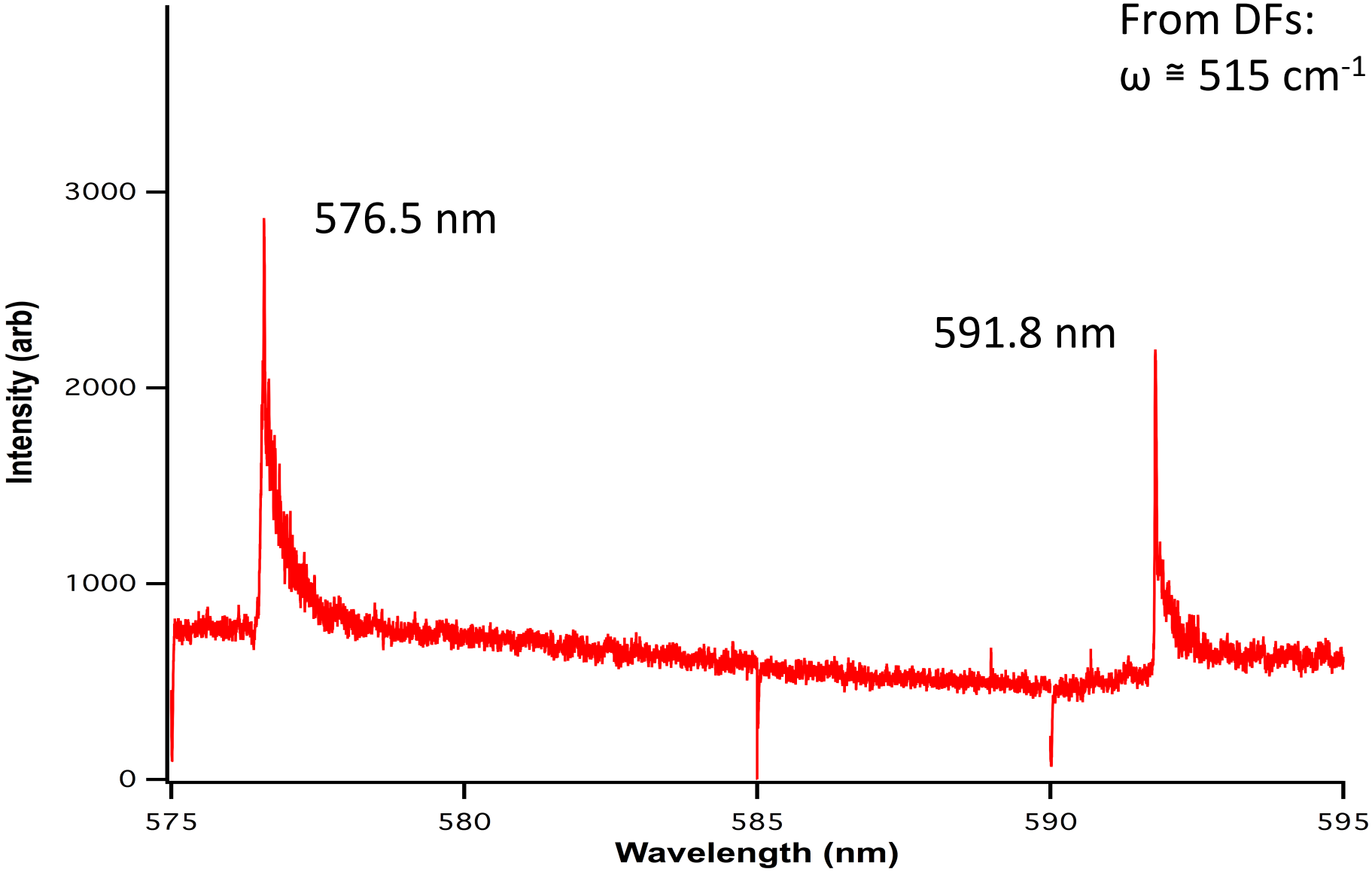
PGOPHER Simulation of $[20.8]^4\Sigma^- - X^4\Sigma^-$



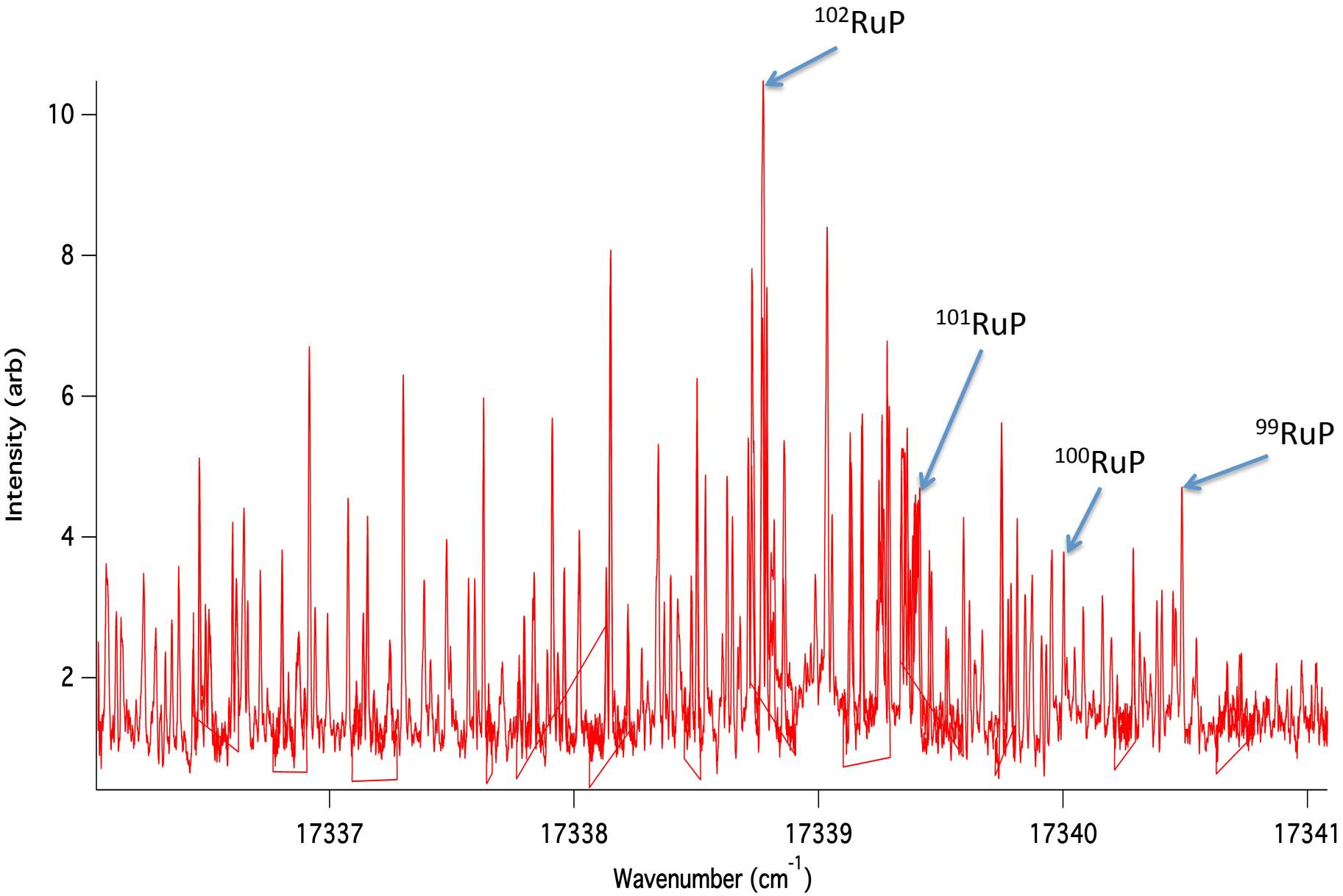
Molecular Constants for RuH

	PGOPHER Fitted Values	Balasubramanian	Difference
B" (cm^{-1})	5.628 ± 0.047	-	-
D" (cm^{-1})	-0.00474 ± 0.0021	-	-
λ_{ss}" (cm^{-1})	-0.8065 ± 0.13	-	-
B' (cm^{-1})	4.914 ± 0.063	-	-
D' (cm^{-1})	-0.0227 ± 0.0024	-	-
λ_{ss}' (cm^{-1})	-13.392 ± 0.25	-	-
Origin (cm^{-1})	20782.8 ± 0.47	11964	8819
R" (Å)	1.732 ± 0.05	1.547	0.185
R' (Å)	1.853 ± 0.06	1.722	0.131

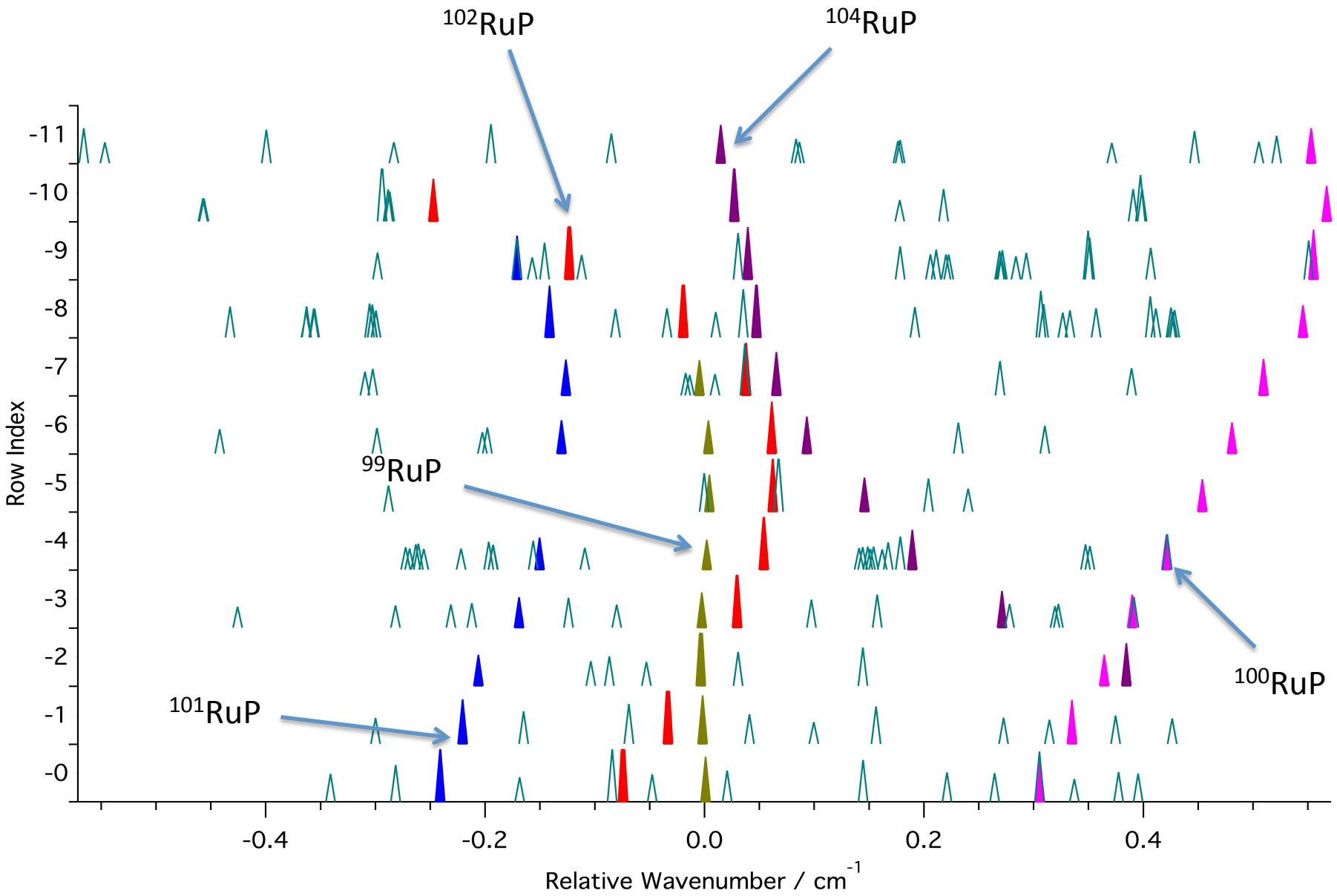
Low Resolution Spectrum of RuP



High Resolution Spectrum of RuP



Loomis-Wood Plot for some branches of RuP



RuP Results

- Numerous branches have been identified for five isotopologues of RuP
- Δ_1F ground state combination differences for ^{102}RuP give integer quantum numbers consistent with a Σ electronic state and yield a B" value of 0.34598 cm^{-1}.
- Upper state combination differences seem to give half-integer quantum numbers but the effective B value is not constant.

Future Work

- Take high resolution data for RuH/D in order to resolve the isotopologues.
- Solve the mystery of the excited state of RuP

Acknowledgements

- Joyce MacGregor, Jacob Dore